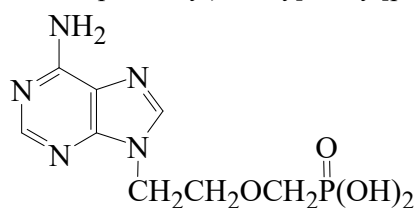




>>Entry Name: Adefovir, BAN, INN, USAN

Synonym(s): 9-[2-(Phosphonylmethoxy)ethyl]adenine. [2-[(6-Amino-9H-purin-9-yl)ethoxy]methyl]phosphonic acid, 9Cl. PME.A. GS 0393



CAS Registry Number: 106941-25-7

Molecular Formula: C₈H₁₂N₅O₄P

Molecular Weight: 273.188

Accurate Mass: 273.062692

Percentage Composition: C 35.17%; H 4.43%; N 25.64%; O 23.43%; P 11.34%

Use/Importance: Potent inhibitor of HIV and related retroviruses. Immunomodulator. Exp. antitumour agent. Congener of Tenofovir [DCY52-Z](#)

Physical Description: Laths (H₂O)

Melting Point: Mp 282-284°

pKa Value: pK_{a1} 4.16; pK_{a2} 6.9

Calculated Log P Data: Log P -1.99 (uncertain value) (calc)

>>Derivative: Mono-Me ester

CAS Registry Number: 107021-27-2

Molecular Formula: C₉H₁₄N₅O₄P

Molecular Weight: 287.214

Percentage Composition: C 37.64%; H 4.91%; N 24.38%; O 22.28%; P 10.78%

Physical Description: Cryst. (EtOH aq.)

>>Derivative: Mono-Et ester

CAS Registry Number: 116384-54-4

Molecular Formula: C₁₀H₁₆N₅O₄P

Molecular Weight: 301.241

Percentage Composition: C 39.87%; H 5.35%; N 23.25%; O 21.24%; P 10.28%

Physical Description: Cryst. (EtOH aq.)

>>Derivative: Di-Et ester

CAS Registry Number: 116384-53-3

Molecular Formula: C₁₂H₂₀N₅O₄P

Molecular Weight: 329.295

Percentage Composition: C 43.77%; H 6.12%; N 21.27%; O 19.43%; P 9.41%

Physical Description: Cryst. (EtOAc/petrol)

Melting Point: Mp 137°

>>Derivative: Bis(2,2-dimethylpropanoyl)ester

Synonym(s): Adefovir dipivoxil, BAN, USAN. GS 0840. Bis-POM-PMEA

CAS Registry Number: 142340-99-6

Molecular Formula: C₂₀H₃₂N₅O₈P

Molecular Weight: 501.475

Accurate Mass: 501.198852

Percentage Composition: C 47.90%; H 6.43%; N 13.97%; O 25.52%; P 6.18%

Use/Importance: Used to increase uptake of adefovir across biological membranes *in vitro* and *in vivo*

Other Data: Prodrug of adefovir. Characterised spectroscopically

References: